

Topological effects, index theorem and supersymmetry in graphene

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Abstract

We present the electronic properties of massless Dirac fermions characterized by geometry and topology on a graphene sheet in this chapter. Topological effects can be elegantly illuminated by the Atiyah-Singer index theorem. It leads to a topological invariant under deformations on the Dirac operator and plays an essential role in formulating supersymmetric quantum mechanics over twisted Dolbeault complex caused by the topological deformation of the lattice in a graphene system. Making use of the G index theorem and a high degree of symmetry, we study deformed energy eigenvalues in graphene. The Dirac fermion results in $SU(4)$ symmetry as a high degree of symmetry in the noninteracting Hamiltonian of the monolayer graphene. Under the topological deformation the zero-energy states emerge naturally without the Zeeman splitting at the Fermi points in the graphene sheet. In the case of nonzero energy, the up-spin and down-spin states have the exact high symmetries of spin, forming the pseudospin singlet pairing. We describe the peculiar and unconventional quantum Hall effects of the $n = 0$ Landau level in monolayer graphene on the basis of the G index theorem and the high degree of symmetry.

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I. INTRODUCTION

Carbon provides a fundamental material for all life and physical science. Carbon-based systems reveal a variety of structures with a great deal of physical properties. These physical properties result from the dimensionality of the structures among systems with carbon atoms. For a long time, in material science, both experimentalists and theorists have sought for the existence of a true two-dimensional (2D) material with the thickness of a single atom, or a membrane of atomic thickness. This 2D material was theoretically first studied on a monolayer of graphite by Wallace [1]. Experimentally in the year 2004, a group led by A. K. Geim at the University of Manchester, U. K., realized such a 2D material under the name of graphene [2, 3].

Graphene is composed of carbon atoms placed at the vertices of a two dimensional honeycomb lattice. It is regarded as a large molecule of carbon atoms which become strongly bound together on the sites of the honeycomb lattice. For each carbon atom on the lattice, three of the four outer electrons get strongly bond with its neighboring atoms by σ orbitals. The $2p_z$ orbital of the fourth electron produces a π bond with a neighboring carbon atom. The σ bonds form the covalent structure with a honeycomb geometry. The bond strength furnishes the flexibility and robustness for the lattice geometry. On the other hand, the π bonds generate the intrinsic electronic structure of graphene. Each π bond yields the half-filled electrons of p orbital to tunnel from a carbon atom to the neighboring one. Thus graphene should be regarded as a many body system on which electrons can get correlated from site to site, resulting in a rich collective behavior. The correlated behavior can be represented by quantum effects which can influence on graphene's electronic properties [2].

The electronic structure can be described by 2D massless relativistic fermions[4–7] in graphene. The massless fermions enable us to study topological effects on electronic properties of graphene. Topological effects are represented by the global properties of geometrical objects rather than their local ones. By varying the geometry, we can produce topologically different configurations such as a sphere or a torus on which the effective Dirac operators of massless fermions are well defined. Described by the Dirac fermions, graphene can have extraordinary properties of stability obtained in terms of geometry and topology of the underlined lattice. Apart from the robust structure of geometry, the topological properties can emerge due to long range quantum coherence in graphene. It follows that we can move

electrons coherently through the whole graphene molecule, resulting in its detection of geometry or topology. This allows us to study a great deal of physical properties revealed by interplay between geometry and topology, and quantum effects[8, 9].

As quantum effects, there exist unconventional quantum Hall effects (QHE) which form a series of filling factors $\nu = \pm 2, \pm 6, \pm 10, \dots$ as the four-fold degeneracy combined by spin and sublattice valley ones [6, 7]. The energy dispersion shows a linear spectrum by the massless Dirac fermions with a Fermi velocity $v_F \approx 10^6 m/s$. The 4-fold degeneracy of the Landau level (LL) is lifted into 4 sublevels in the presence of an external high magnetic field. In the case of the tilted high magnetic field to the graphene plane, the spin degeneracy can be lifted at the first LL, resulting in the filling factor $\nu = 4$ QHE of monolayer graphene [10]. Furthermore for bilayer graphene, the LL spectrum is composed of eightfold degenerate states at the zero energy and fourfold ones at finite energies under the high magnetic field. This can allow us to observe the quantum Hall plateaus at a series of $\nu = \pm 4, \pm 8, \pm 12, \dots$ [11–13]. The charge carriers are chiral massive fermions which produce a parabolic energy band. The chiral fermions offer the unconventional integer QHE of the zero-LL anomaly which exhibits metallic behavior under the condition of low carrier densities and high magnetic fields in contrast to the conventional insulating phenomena [6, 7, 9–14].

Topological configurations can produce a crucial effect on the quantum states of a system. In particular, they can provide the possible quantum ground states which a system can have. This remarkable result is described in terms of the index theorem initiated by Atiyah and Singer [15]. It gives the relationship between the analytic properties of the operator and the topological characteristic of the manifold upon which the operator is defined. The Dirac operator can be related to topological effects which is elegantly illuminated by the Atiyah-Singer index theorem in graphene [8]. It leads to a topological invariant under deformations on a Dirac operator and plays an essential role in formulating supersymmetric quantum mechanics (SUSY QM) on the graphene sheet [9, 16].

In a theoretical sense, there has been at least the quantum mechanics (QM) of particles described by both fermionic and bosonic degrees of freedom. The SUSY QM may be hidden in the quantum mechanics of a particle acting on a group manifold which can be represented by a high degree of symmetry [17]. As an example, a spin precessing in a magnetic field can have the hidden SUSY. In particular, under the uniform magnetic field the LL for an electron can be expressed by the spectrum of the SUSY oscillator which is composed of

fermionic and bosonic ones. It is remarkable that this SUSY QM can possibly emerge in graphene with low carrier concentration and high mobility. The supersymmetry is built up over the Dolbeault complex due to the topological deformation on the lattice in a graphene system [9, 17, 18].

We exploit the G-index theorem and a high degree of symmetry to understand unusual quantum Hall effects of the $n = 0$ Landau level in graphene. The Dirac fermion results in $SU(4)$ symmetry as a high degree of symmetry in the noninteracting Hamiltonian of the monolayer graphene. The high symmetries in graphene sheets can not couple to an external magnetic field. In the absence of the magnetic field the index theorem can provide a relation between the zero-energy state of the graphene sheet and the topological deformation of the compact lattice. Under the topological deformation the zero-energy states emerge naturally without the Zeeman splitting at the Fermi points in the graphene sheet. In the case of nonzero energy, the up-spin and down-spin states have the exact high symmetries of spin, forming the pseudospin singlet pairing. We describe the peculiar and unconventional quantum Hall effects of the $n = 0$ Landau level in monolayer graphene on the basis of the index theorem and the high degree of symmetry [9, 18].

This chapter is written as follows. We explain basic properties of graphene in section II. In section III, we discuss a path integral of coherent states in brief. In section IV, supersymmetry is introduced in graphene. In the following section, we investigate the Atiyah-Singer index theorem and topological properties. The G index theorem and deformation is covered. In section VI, SUSY QM and higher spin symmetry are described. Next we illuminate the low energy spectrum and unconventional quantum Hall effects in monolayer graphene. And finally we come to summary and conclusion.

II. BASIC PROPERTIES OF GRAPHENE

Graphene is a molecule that is composed of carbon atoms placed on a two dimensional honeycomb lattice. The basic plaquette of the lattice has a hexagon and the atoms are located at the sites of the lattice. Electronic properties of graphene can be described by the tight binding model on which spinless electrons move from site to site along the links of the lattice without interaction each other. Under the tight-binding approximation graphene can be expressed by a simple Hamiltonian of coupled fermions on a hexagonal lattice [2, 19].

The model Hamiltonian is a form given by

$$H = -\frac{2v_F}{3} \sum_{\langle i,j \rangle} c_i^\dagger c_j, \quad (1)$$

where $\langle i, j \rangle$ indicates nearest neighbors on the lattice. c_i^\dagger and c_i are the creation and annihilation operators of the fermions located at site i with anticommutation relation $\{c_i, c_j^\dagger\} = \delta_{ij}$.

In order to calculate the spectrum of Hamiltonian (1), we account for a periodicity of honeycomb lattice which leads to a Fourier transformation. The periodic structure provides the energy eigenvalue problem for the Hamiltonian in a unit cell. The unit cell consists of two neighboring carbon atoms called A and B . They can be expressed by the three vectors $\vec{u}_i, \forall i = 1, 2, 3$. Under the Fourier transformation of $c(\vec{p}) = \sum_i e^{i\vec{p} \cdot \vec{u}_i} c_i$, the Hamiltonian is rewritten in terms of

$$H = -\frac{2v_F}{3} \int \int d^2p \left(c_A^\dagger(\vec{p}), c_B^\dagger(\vec{p}) \right) \begin{pmatrix} 0 & \sum_{i=1}^3 e^{i\vec{p} \cdot \vec{u}_i} \\ \sum_{i=1}^3 e^{-i\vec{p} \cdot \vec{u}_i} & 0 \end{pmatrix} \begin{pmatrix} c_A(\vec{p}) \\ c_B(\vec{p}) \end{pmatrix}, \quad (2)$$

where $c_A(\vec{p})$ and $c_B(\vec{p})$ denote the Fourier transformed operators corresponding to the carbon atoms A and B , respectively.

Now it is easy to take the eigenvalue of the energy for electrons of graphene. The dispersion energy is given by [8, 9, 19]

$$E(p) = \pm \frac{2v_F}{3} \sqrt{1 + 3 \cos^2 \frac{\sqrt{3}p_y}{2} + 4 \cos \frac{3p_x}{2} \cos \frac{3p_y}{2}} \quad (3)$$

where the lattice distance between atoms becomes normalized to the unity. From the dispersion relation obtained above, graphene can have two independent Fermi points, $\vec{p} = K_\pm = \pm \frac{2\pi}{3}(1, \frac{1}{\sqrt{3}})$. We can expand it and then linearize it near the conical singularities of the Fermi points. Corresponding to the K_+ and K_- at the half-filling case, the Hamiltonian is expressed by the Dirac operators

$$H^\pm = \pm v_F \sum_{\mu=x,y} \gamma^\mu p_\mu, \quad (4)$$

where $p_\mu = -i\hbar\partial_\mu$ is the covariant momentum and the Dirac matrices γ^μ indicate the Pauli matrices $\gamma^\mu = \sigma^\mu$. Hence the low energy theory of graphene is described by means of free fermions.

The Hamiltonian can be written in the matrix form [8, 9]

$$H^\pm = \begin{pmatrix} 0 & D_\pm \\ D_\pm & 0 \end{pmatrix}. \quad (5)$$

Here D_\pm is a Dirac operator given by

$$D_\pm = \pm v_F(\sigma^x p_x + \sigma^y p_y), = \mp 2i\hbar v_F \begin{pmatrix} 0 & \partial_z \\ \partial_{\bar{z}} & 0 \end{pmatrix}. \quad (6)$$

Here we have expressed D_\pm in terms of $\partial_z = \frac{1}{2}(\partial_x - i\partial_y)$ and $\partial_{\bar{z}} = \frac{1}{2}(\partial_x + i\partial_y)$. On the complex coordinates we can write

$$\nabla^2 = 4\partial_z\partial_{\bar{z}}. \quad (7)$$

So far, we have discussed the collective behavior of graphene electrons that can be governed by the Dirac equation. In particular, the velocity of the electrons is effectively 300 times smaller than the speed of light.

Next let us describe a curved graphene. On the curved surface of graphene the low energy physics can be illuminated by the Dirac equation that is defined on the corresponding curved manifold. The curvature generates an gauge field of magnetic flux going through the curved graphene. This yields to a picture about how to interact gauge fields with Dirac fermions. In order to have the way associated with the gauge fields, let us take into account a good method to include curvature to graphene. The simplest way is that we cut a $\frac{\pi}{3}$ piece of triangle from a graphene sheet and then gluing the opposite ends of the lattice. This process results in a single pentagon at the apex of the generated cone while all the other plaquette keep a hexagon. Due to the minimal geometrical distortion, the honeycomb lattice has a positive curvature. The curvature can be obtained by calculating a circular tangent vector, V , around the apex by $\oint V \cdot d\vec{r} = \frac{\pi}{3}$. The generation of a single pentagon gives rise to a dramatic effect on the spinor, resulting in deformation of the lattice. If the spinor is parallel transported around the apex by an angle 2π , it is forced at some point to make a jump from a site A to a site A while every site A takes only B neighborhoods or vice versa. This motion enables us to have the effect that the magnetic field gives on the wave function of a particle moving on a closed path. A full circulation provides accumulation of all phase factors to the particle wave function, and so generates the enclosed magnetic flux. This flux allows us to observe the Aharonov Bohm effect. Quantum mechanically, it can provide a

discontinuity. Thus we have simultaneously to describe it through the wave function of the particle in the processes of being static or moving along the closed trajectory. This produces a vector potential term in the Hamiltonian that leaves the theory to be consistent.

By similar procedures made on the curved graphene that compensates the jump in the components of the spinor, we should take into account a nonabelian vector potential A in the effective Hamiltonian. Around the apex we can take the circulation of A along a path. It is expressed by $\oint_{\gamma} A \cdot d\vec{r} = \frac{\pi}{2}\tau_2$, where τ_2 denotes the second Pauli matrix which couples the K_+ to the K_- components of the spinor. The effective gauge theory can be emerged due to the geometric deformation on geometric variants of graphene as topological effects. In next section we describe a path integral of the coherent states for geometrical and topological properties.

III. PATH INTEGRAL OF COHERENT STATES

Let us construct a path integral of the coherent states on a group manifold. Following the Stone's approach [17], we discuss the coherent states on a general group G . Let us take $D(g)$, any $g \in G$, as an irreducible representation of the group. Assume that $|0\rangle$ is some state in the space of representation. Then one can define $|g\rangle$ by

$$|g\rangle = D(g)|0\rangle. \quad (8)$$

On the basis of the irreducible representation, Shur's lemma holds that

$$\frac{1}{V(G)} \int d[g] |g\rangle\langle g| = 1 \quad (9)$$

where $\frac{1}{V(G)}$ is the volume of the group manifold. In the expression of Eq. (9) $d[g]$ is the Haar measure on the group.

Let us compute a thermodynamic partition function

$$Z = \text{Tr}(e^{-\beta H}) \quad (10)$$

where β is the imaginary time. In the procedure of calculating the partition function, the trace is constrained to the representation space on which $D(g)$ acts. Dividing the Matsubara time-interval β into n parts, and using the Shur's lemma of Eq. (9), we can write down an iterated integral

$$\text{Tr}(e^{-\beta H}) = \text{const.} \int (d[g]d[g'] \cdots) \langle g|e^{-\beta H/n}|g'\rangle \langle g'|e^{-\beta H/n} \cdots |g\rangle. \quad (11)$$

where const. is the constant value taken on the representation space. When taking into account short time intervals, one can express $g' \simeq g + \delta g$, and $\delta g \simeq O(\delta t)$, so that

$$\begin{aligned} & \langle g | e^{-\delta t H} | g' \rangle \\ & \approx 1 + \langle g | \delta g \rangle + \langle g | (-\delta t H) | g \rangle + O(\delta t^2). \end{aligned} \quad (12)$$

On taking into consideration up to order $O(\delta t)$, we can write down the formal path-integral expression

$$\begin{aligned} & \text{Tr}(e^{-\beta H}) \\ & = \frac{1}{V(G)} \int d[g] \exp(\oint \langle g | \delta g \rangle - \int_0^\beta dt \langle g | H | g \rangle). \end{aligned} \quad (13)$$

Here $d[g]$ is regarded as the path-integral measure given by the Haar measure at each time step.

The path-integral expression can be identified as a path integration over a quotient space of the group. In particular it is noted that a set of the $|g\rangle$ can be different from only a phase so that the integrand is not sensitive to the phase factor. Now suppose that H is the subgroup of G , constructed from exponentiating a maximal commuting set of generators, i.e., a maximal torus. Then $|0\rangle$ is expressed by an eigenstate of the generators of H which means a state of definite weight. The $|g\rangle$ are represented by all phase multiples of one another in any one coset of G/H . And hence the coherent states can be described in terms of a bundle over G/H with the maximal torus as the gauge group, and the integration is made over the path in G/H .

Let us express the integrand in the coherent-state path integral without any choice of representatives. In order to make a natural procedure on the independent choice of the representatives, we define the projection operators as

$$P(g) = |g\rangle \langle g|. \quad (14)$$

They can be directly projected onto the physically distinct states since they do not have any phase ambiguity. In the integrand, the first term $\oint \langle g | \delta g \rangle$ can be taken to be a gauge invariant form by using Stokes theorem

$$\oint_{\Gamma=\partial\Omega} \langle g | dg \rangle = \int_{\Omega} d \langle g | dg \rangle. \quad (15)$$

Making use of the identity form

$$d \langle g | dg \rangle = \langle dg | dg \rangle = -\text{Tr}(dPPdP), \quad (16)$$

the first term yields

$$\oint_{\Gamma=\partial\Omega} \langle g|dg \rangle = - \int_{\Omega} \text{Tr}(dPPdP). \quad (17)$$

The second term in the integrand can be rewritten by

$$\langle g|H|g \rangle = \text{Tr}(P(g)H). \quad (18)$$

Hence combination of Eqs. (17) and (18) leads us to the path integral given by [17]

$$\text{Tr}(e^{-\beta H}) = \frac{1}{V(G/H)} \int d[g] \exp \left(- \int_{\Omega} \text{Tr}(dPPdP) - \int_{\Gamma} \text{Tr}(P(g)H) \right). \quad (19)$$

It is noted that the elements of G/H can only contribute to the integrand, so that the volume factor of the gauge group H gets out of the path integral.

There are certain subgroups corresponded to the Lie algebra \mathcal{G} of a Lie group G . Let us describe some basic facts about semisimple Lie algebra in brief. Then it is known that the generators of the \mathcal{G} can have a decomposition into a maximally commuting set $\mathcal{H} = \{H_i\}$, i.e., the Cartan subalgebra, and a set of ladder operators, E_{α} , one for each root vector $\alpha \in R$. The ladder operators are needed for complexifying the algebra to \mathcal{G}^c which results from the group parameters to get the complex values. The H_i and the E_{α} hold that

$$[H_i, E_{\alpha}] = \alpha_i E_{\alpha}. \quad (20)$$

Assume that $|\lambda \rangle$ is an eigenvector of the H_i with eigenvalues λ_i such as

$$H_i |\lambda \rangle = \lambda_i |\lambda \rangle. \quad (21)$$

Then

$$E_{\alpha} |\lambda \rangle = |\lambda + \alpha \rangle. \quad (22)$$

The roots may be classified into two sets by an arbitrary hyperplane on a root space. On one set the root objects are positive roots indicated by $\alpha \in R_+$ as increasing the weights while the others are negative roots, by $\alpha \in R_-$ as decreasing the weights. And thus we can take the greatest weight as a state which is annihilated by all $E_{\alpha}, \alpha \in R_+$.

This decomposition of the Lie algebra is made on some kinds of special subgroup. The Borel subgroups B_{\pm} are constructed by exponentiating the algebras \mathcal{B}_{\pm} which are spanned by the $E_{\alpha}, H_i; \alpha \in R_{\pm}, H_i \in \mathcal{H}^c$. Any $g \in G$ can be decomposed into the gaussian factors

$$g = \zeta_- h \zeta_+; \quad \zeta_- \in Z_-, \zeta_+ \in Z_+, h \in H_+^c, \quad (23)$$

where the Z_{\pm} are the groups obtained by exponentiating the $E_{\alpha}, \alpha \in R_{\pm}$. As an example, the gaussian factor ζ_{-} can be written as

$$\zeta_{-} = \exp\left(\sum_{\alpha \in R_{-}} z^{\alpha} E_{\alpha}\right). \quad (24)$$

When the representation matrix $D(g)$ is applied to a greatest weight, the factor ζ_{+} is regarded as the identity. The z^{α} can be taken as complex coordinates for the coset space G^c/B_{+} . It follows that the set of physically distinct states can have an one-to-one correspondence to the G^c/B_{+} . For a complex manifold we can choose complex coordinates on the manifold with holomorphic functions. And constructed on non-greatest weight states, coherent states are described by nonholomorphic functions of \bar{z} . In the next section, after introducing supersymmetry on the complex manifold in brief, we will describe supersymmetric quantum mechanics in graphene [9, 16].

IV. SUPERSYMMETRY IN GRAPHENE

Let us use the methods of Witten to introduce fermionic creation operators $\psi^{x\dagger}$ and $\psi^{y\dagger}$ which correspond to the differential forms dx and dy [9, 16]

$$dx \leftrightarrow \psi^{x\dagger}|0\rangle, \quad dy \leftrightarrow \psi^{y\dagger}|0\rangle. \quad (25)$$

In more detail $\psi^{x\dagger}$ performs the operation of exterior multiplication by dx while the adjoint, ψ_x , does that of interior multiplication by the vector dual to dx , say, ∂_x

$$\iota : \partial_x \rightarrow \psi_x, \quad \mathcal{E} : dx \rightarrow \psi^{x\dagger}, \quad \iota : \partial_y \rightarrow \psi_y, \quad \mathcal{E} : dy \rightarrow \psi^{y\dagger}. \quad (26)$$

The fermionic operators satisfy the anticommutation relations

$$\{\psi_{\mu}, \psi^{\nu\dagger}\} = \delta_{\mu}^{\nu}, \quad \mu, \nu = x, y. \quad (27)$$

On the basis of these definitions let us set up

$$\frac{1}{2}(\psi_x - i\psi_y) = \psi_z = \frac{1}{2}\psi^{\bar{z}}, \quad \frac{1}{2}(\psi_x + i\psi_y) = \psi_{\bar{z}} = \frac{1}{2}\psi^z. \quad (28)$$

while holding the Hermitian conjugate relations.

Now let us describe a supersymmetry over the complex Kähler manifold. On the complex manifold we take two supercharges

$$\begin{aligned} Q_1 &= \partial = \psi^{\dagger z} \partial_z, \quad Q_1^\dagger = \bar{\partial} = -\psi^{\bar{z}} \partial_{\bar{z}}, \\ Q_2 &= \bar{\partial} = \psi^{\dagger \bar{z}} \partial_{\bar{z}}, \quad Q_2^\dagger = \partial = -\psi^z \partial_z. \end{aligned} \quad (29)$$

Making use of anticommutation relations for fermions, these supercharge operators allows us to express

$$\begin{aligned} \partial \bar{\partial} + \bar{\partial} \partial &= Q_1 Q_1^\dagger + Q_1^\dagger Q_1 = -\frac{1}{2} \nabla^2, \\ \bar{\partial} \partial + \partial \bar{\partial} &= Q_2 Q_2^\dagger + Q_2^\dagger Q_2 = -\frac{1}{2} \nabla^2. \end{aligned} \quad (30)$$

Here it is easy to check that the cross terms such as

$$\partial \bar{\partial} + \bar{\partial} \partial = Q_1 Q_2^\dagger + Q_2^\dagger Q_1 = 0, \quad (31)$$

do not have any contributions.

In terms of the two supercharge operators, the Dirac operators D_\pm in graphene is given by

$$D_\pm = \mp i \hbar v_F (Q_1 + Q_2), \equiv Q_\pm. \quad (32)$$

The Dirac operators can be described by means of the sum of the two supercharges which is the ordinary exterior derivative, d . And Q_\pm become the supercharge of $N = 1$ supersymmetric quantum mechanics. It is not hard to check up that $D_\pm = Q_\pm + Q_\pm^\dagger$ is given by

$$Q_\pm + Q_\pm^\dagger = \mp 2i \hbar v_F \begin{pmatrix} 0 & \partial_z \\ \partial_{\bar{z}} & 0 \end{pmatrix} \quad (33)$$

which are equivalent to Eq. (6). Furthermore the square of Eq. (33) can lead to

$$(Q_\pm + Q_\pm^\dagger)^2 = -4(\hbar v_F)^2 \begin{pmatrix} \partial_z \partial_{\bar{z}} & 0 \\ 0 & \partial_{\bar{z}} \partial_z \end{pmatrix} = -\hbar^2 v_F^2 \nabla^2, \quad (34)$$

where we have exploited Eq. (7). And hence in the sense of SUSY QM the Hamiltonian of graphene may be recapped in terms of the following form

$$H \equiv 2(Q_\pm + Q_\pm^\dagger)^2 = -2\hbar^2 v_F^2 \nabla^2, \equiv -\frac{\hbar^2 \nabla^2}{2m^*}, \quad (35)$$

provided that the mass, m^* were defined by $m^* = \frac{1}{4v_F^2}$ in the last expression of the eq. (17). The Witten index is given by

$$\text{Index(d)} = \text{Tr} \left((-1)^F e^{-tH} \right) \quad (36)$$

which accounts for the Euler number of the manifold as the exterior calculus of the de-Rham complex. In order to build up the supersymmetry over the Dolbeault complex [22], we need one of the supercharges, $Q_2 = \bar{\partial}$. On the manifold of real dimension $2n$, the index of the Dolbeault complex is given by

$$\text{Index}(\bar{\partial}) = \text{Tr} \left((-1)^F e^{-t(Q_2 + Q_2^\dagger)^2} \right) \quad (37)$$

This index is more interested in the the SUSY QM over twisted Dolbeault complex which is associated with deformation of the topology of the lattice on a graphene system . And in the next section we build the Atiyah-Singer and G index theorem as well as the energy eigenvalues on the deformation of the compact manifold.

V. INDEX THEOREM IN GRAPHENE

Let us describe the index theorem which gives an insight on the spectrum structure of certain operators such as the Dirac operators. In graphene this theorem enables us to have physical properties associated with the topology and geometry of the space in which the Dirac operators are defined. It provides the relationship between the analytic properties of the operator and the topological characteristics of the manifold.

A. The Atiyah-Singer index theorem in graphene

We illuminate the Atiyah-Singer index theorem by the method employed to the heat kernel expansion. The theorem furnishes a relation between zero eigenvalues of the Dirac operator of graphene and the total flux which goes through its surface. If the latter is connected to the genus of the surface through the Euler characteristic, we can find a close relation between the zero modes and the topology of the surface on a graphene system.

Let us start with a Dirac operator given by

$$K = \begin{pmatrix} 0 & D^\dagger \\ D & 0 \end{pmatrix}. \quad (38)$$

Here D means an operator that maps a space M_+ onto a space M_- while D^\dagger is a map from M_- to M_+ . If D is an $n \times m$ matrix, D^\dagger becomes a $m \times n$ matrix. M_+ and M_- are the space of n and m dimensional vectors, respectively. Because we are focusing on the zero modes of K such that the solutions of the equations $K\Psi = 0$, let us define the number of different eigenstates of D with zero eigenvalue as η_+ and the ones of D^\dagger as η_- . As a bookkeeping of chirality, the chirality operator γ_5 is defined as

$$\gamma_5 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (39)$$

Its eigenstates can have eigenvalue \pm provided that they act on M_\pm .

In order to calculate the number of zero eigenstates in which we are interested, we take into account the operator K^2 that has the same number of zero modes as K . The K^2 can be given by a diagonal form

$$K^2 = \begin{pmatrix} D^\dagger D & 0 \\ 0 & DD^\dagger \end{pmatrix}. \quad (40)$$

It is claimed that the operators $D^\dagger D$ and DD^\dagger get the same non-zero eigenvalues. To prove this statement, assume that $DD^\dagger\psi = \lambda\psi$ for eigenvalue $\lambda \neq 0$. Then it follows that

$$DD^\dagger\psi = \lambda\psi \longrightarrow D^\dagger D(D^\dagger\psi) = \lambda(D^\dagger\psi). \quad (41)$$

This means that the operator $D^\dagger D$ gives the same eigenvalue, λ , which corresponds to the eigenstate $D^\dagger\psi$. But it is not necessary to hold the case for $\lambda = 0$ when $D^\dagger\psi$ might be zero by itself.

Let us compute the trace of $\gamma_5 e^{-tK^2}$ as followings:

$$\text{Tr}(\gamma_5 e^{-tK^2}) = \text{Tr}(e^{-tD^\dagger D}) - \text{Tr}(e^{-tDD^\dagger}) = \sum_{\lambda_+} e^{-t\lambda_+} - \sum_{\lambda_-} e^{-t\lambda_-}, \quad (42)$$

where λ_+ and λ_- indicate the eigenvalues of the operators $D^\dagger D$ and DD^\dagger , respectively, and t is an arbitrary parameter. In the first step of the above procedures, γ_5 acts on the exponential so that it provides a $+1$ to the eigenvectors of $D^\dagger D$ when they are placed in M_+ , and a -1 to the ones of DD^\dagger when they belong to M_- . In the last step the trace is evaluated by a sum over all the eigenvalues of the corresponding operators. Every non-zero eigenvalue of $D^\dagger D$ is a one-to-one correspondence to an eigenvalue of DD^\dagger . Therefore all

paired terms of non-zero eigenvalues cancel out each other. There are left over the zero eigenvalues of each operators, resulting in

$$\text{Tr}(\gamma_5 e^{-tK^2}) = \eta_+ - \eta_-. \quad (43)$$

In general we cannot determine difference between the number of zero modes. It is seen that the above result is independent of t owing to the cancelation of the non-zero eigenvalue term.

Actually we should evaluate $\text{Index}(K)$. In order to calculate it practically, we take an alternative method of heat expansion for calculating $\text{Tr}(\gamma_5 e^{-tK^2})$. It says that for general $\hat{\Gamma}$ and \hat{D} on a two dimensional compact manifold we can expand

$$\text{Tr}(\hat{\Gamma} e^{-t\hat{D}}) = \frac{1}{4\pi t} \sum_{l \geq 0} t^{\frac{l}{2}} b_l(\hat{\Gamma}, \hat{D}), \quad (44)$$

where Tr indicates the trace of matrices and the integration over coordinates of space. b_l denote expansion coefficients. For $\hat{\Gamma} = \gamma_5$ and $\hat{D} = K^2$, we have to return to an expression that is t -independent. For this t -independence, the expansion coefficients should vanish for all l except for $l = 2$ under the condition that all the t contributions is canceled out each other. This allows us to determine the coefficient b_2 from the first order term in t in the series of expansion. For the evaluation, let us take D as $D = -ie_\nu^\mu \sigma^\nu (\nabla_\mu - ieA_\mu)$. Here e_ν^μ indicates the zweibein of curved surface metric $g_{\mu\nu}$ that defines a local flat frame $\eta_{\alpha\beta} = e_\alpha^\mu e_\beta^\nu g_{\mu\nu}$ while σ_μ is the Pauli matrix. A_μ denotes a gauge field. It follows that

$$K^2 = -g^{\mu\nu} \nabla_\mu \nabla_\nu + \frac{1}{4} [\gamma^\mu, \gamma^\nu] F_{\mu\nu} - \frac{1}{4} R \quad (45)$$

where R is curvature, and $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ means the field strength. ∇_μ indicates a covariant derivative with respect to gauge and reparametrization transformation.

It is easy to see that the non-zero expansion coefficient b_2 is written by

$$b_2 = \text{Tr}[\gamma_5 (\frac{i}{4} [\gamma^\mu, \gamma^\nu] F_{\mu\nu} - \frac{1}{4} R)] = 2 \int \int B \cdot dS, \quad (46)$$

where B is the magnetic field given by $B_l = \frac{1}{2} \epsilon^{l\mu\nu} F_{\mu\nu}$. The integration has been over the whole surface. These two independent ways for calculating $\text{Tr}(\gamma_5 e^{-tK^2})$ allows u to arrive at the final formula of the index theorem [8]

$$\text{Index}(K) = \nu_+ - \nu_- = \frac{1}{2\pi} \int \int B \cdot dS. \quad (47)$$

It states that the total flux which goes out of the surface is related to the number of zero modes of the K operator. The curvature doesn't contribute to the index formula because γ_5 is a traceless operator. Particularly no contribution of curvature is to show an intrinsic property of two dimensional surfaces. The index theorem leads to an integer number on the compact surfaces. Therefore $\int \int \mathbf{B} \cdot d\mathbf{S}$ produces the total magnetic monopole charge in discrete values inside the surface under the Dirac quantization condition of magnetic monopoles.

Using the index theorem, we observe the topological characteristics of graphene. Let us apply it to graphene and its geometric variants. In a certain configuration of graphene we have to account for the effective magnetic field on the graphene surface. Some plaquette deformations give rise to a specific circulation of the vector potential around a loop trajectory. Stokes's theorem helps us to have a relation between the circulation of the gauge potential around a loop γ_i and the flux of the corresponding magnetic field

$$\oint_{\gamma_i} \mathbf{A} \cdot d\vec{r} = \int \int_{S_i} \mathbf{B} \cdot d\mathbf{S}, \quad (48)$$

where S_i indicates the area. Hence going through the surface of graphene the total flux can be obtained from the fact that we can know the total number of deformations. It is necessary for us to have some information about the total number of plaquette deformations. The information is related to the topological properties of the surface through the Euler characteristics. Let us consider the Euler theorem in the following subsection.

B. Euler theorem

In general the Euler theorem gives rise to a relation between the structural information of a polyhedral lattice and its topological properties. There are a lot of proofs on this theorem. The most common methods are proofs on the basis of a reductions from the polyhedral lattice to the simpler one without changing its topological properties.

Let us consider a lattice placing on a compact surface with a certain genus g . Then we can compute the number of deformations in a lattice necessary to create such a surface by applying the Euler characteristic. Let V, E and F be the number of vertices, edges and faces of the lattice, respectively, and N_{end} , open ends. Then the Euler characteristic, χ is

expressed by [8]

$$\chi = V - E + F = 2(1 - g) - N_{end}. \quad (49)$$

The second step of Eq. (49) is satisfied by the Euler theorem. It is easily to check that a single cut in the surface can have a reduction of the genus by one and increase the number of open ends by two, say, $(g, N_{end}) \rightarrow (g - 1, N_{end} + 2)$, leaving the Euler characteristic χ preserved.

Let us apply the Euler theorem to the case of graphene molecules. There are three links on each vertex of graphene. Suppose that topological deformations such as pentagons or heptagons are present. Let us indicate the total number of pentagons, hexagons and heptagons by n_5, n_6 and n_7 , respectively in the molecule. Then the total number of vertices is written by $V = (5n_5 + 6n_6 + 7n_7)/3$ when each k -gon has k vertices and each vertex takes three polygons. Similarly, the total number of edges is expressed by $E = (5n_5 + 6n_6 + 7n_7)/2$ provided that each edge has two polygons. The total number of faces is equal to the sum of different polygons, $F = n_5 + n_6 + n_7$. Combining these into the Euler characteristic, we see that

$$n_5 - n_7 = 6\chi = 12(1 - g) - 6N_{end}. \quad (50)$$

This result reflects many facts. When equal numbers of pentagons and heptagons are inserted, they do not make any change about the topology of the surface in the case that they cancel out. On a flat graphene sheet we can put two pentagons and two heptagons on it without changing the curvature of the molecule away from these deformations. This is consistent with the effective gauge flux approaches where pentagons and heptagons give opposite flux contributions. On the other hand, it is known that nontrivial topologies necessarily provide an imbalance between pentagons and heptagons. The genus zero configurations result in an excess of pentagons while high genus surface has an excess of heptagons. Genus one surfaces do not have any pentagons or heptagons at all provided that they are equivalent to a flat sheet.

It is seen that Eq. (50) recaps the known result of a sphere with $g = 0$ which leads to $\chi = 2$. This corresponds to a fact about $n_5 = 12$ and $n_7 = 0$ for the C_{60} fullerene. For a torus with $g = 1$, we can have $\chi = 0$ related to $n_5 = n_7 = 0$ in the case of the nanotubes. Thus no pentagons or heptagons may be required. If we account for the genus $g = 2$ surfaces,

then we can obtain $\chi = -2$ where $n_5 = 0$ and $n_7 = 12$. In this situation equal numbers of pentagons and heptagons can be inserted without making any change of topology on the surface.

Suppose that K is a Dirac Hamiltonian H . Then we compute the $\text{Index}(H)$. The Euler characteristic term allows us to compute the gauge field term in the $\text{Index}(H)$. It can be given by including additionally the contributions from the surplus of pentagons or heptagons. Hence the total flux of the effective gauge field can lead to

$$\begin{aligned}\text{Index}(H) &= \frac{1}{2\pi} \int \int_{S_i} \mathbf{B} \cdot d\mathbf{S} = \frac{1}{2\pi} \sum_{n_5 - n_7} \oint_{\gamma_i} \mathbf{A} \cdot d\vec{r} \\ &= \frac{1}{2\pi} \pi (n_5 - n_7) = 3(1 - g) - \frac{3}{2} N_{end}.\end{aligned}\tag{51}$$

The total number of zero modes is equivalent to the sum contributed from each subsector of a Dirac operator. As a consequence, by adding the two contributions, we arrive at the index of the Dirac Hamiltonian that describes the graphene molecule. The $\text{Index}(H)$ is expressed by [8]

$$\text{Index}(H) = \nu_+ - \nu_- = 6(1 - g) - 3N_{end}\tag{52}$$

which is consistent with the exact number of the zero modes if $\nu_+ = 0$ or $\nu_- = 0$. Therefore we have obtained the theorem which relates the number of zero modes existed in a certain graphene molecule to the topological characteristics of its surface.

This result provides the number of zero modes for the familiar cases of graphene molecules. For example, since a fullerene takes $g = 0$ and $N_{end} = 0$, it is expected that it has six zero modes which correspond to the two triplets of C_{60} and of similar large molecules. For the case of nanotubes, we have $g = 0$ and $N_{end} = 0$. This results in $\nu_+ - \nu_- = 0$ which is in agreement with previous theoretical and experimental results [20, 21]. The index theorem gives rise to a surprising relation between the topology and the presence of magnetic flux which is effectively inserted in graphene molecules by geometrical deformations. The number of these deformations can be associated with the general topological characteristics of the lattice surface. They are related to the zero modes of a general graphene molecule with the genus and the number of open faces of its surface.

C. G index theorem

To build up supersymmetry over the Dolbeault complex which are associated with deformation on topology of the lattice [22], we need one of the supercharges, $Q_2 = \bar{\partial}$. The index theorem leads to a topological invariant under deformations on Q_2 and plays an essential role in formulating the SUSY QM over the twisted Dolbeault complex caused by the deformation in a graphene system.

Let us describe the general statement of the G-index theorem. Suppose that Q and Q^\dagger are supercharges which have a map from a space of bosonic states to a space of fermionic states and vice versa. Further let us take a Lie group G generated by G_i . G_i satisfy the commutation relations with Q and Q^\dagger such that [17]

$$[G_i, G_j] = if_{ij}^k G_k, \quad [Q, G_i] = 0, [Q^\dagger, G_i] = 0, \quad (53)$$

f_{ij}^k are structure constants. G_i has also a commutation relation with the Hamiltonian of Eq. (5)

$$[G_i, H] = 0. \quad (54)$$

A supercharacter can be expressed as a supertrace of the group elements

$$\Xi(e^{i\theta^i G_i}) = \text{Tr} \left((-1)^F e^{i\theta^i G_i} e^{-tH} \right). \quad (55)$$

The ordinary trace requires us to take a limit of $t \rightarrow 0$. But Eq. (55) does not have any dependence on t because the non-zero energy levels can not make contributions due to canceling in pairs between the bosonic and fermionic sectors. But the zero-energy levels can only give contributions. And these are not dependent on t .

The character is topologically invariant under deformations of the operators Q and Q^\dagger . On deformation let us consider the supersymmetry generator Q of the ordinary $N = 1$ SUSY QM on a manifold. In locally geodesic coordinates Q is expressed by

$$Q = d = \psi^{\mu\dagger} \partial_\mu. \quad (56)$$

When deforming Q , it is changed into the new operator

$$Q_s = d + s\iota_K = \psi^{\mu\dagger} \partial_\mu + sK^\mu \psi_\mu, \quad (57)$$

where \mathcal{K} denotes a Killing vector field. And then the deformed Hamiltonian is given by

$$\begin{aligned} H_s &\equiv 2(Q_s + Q_s^\dagger)^2, \\ &= -\partial^2 + s^2|\mathcal{K}|^2 - \frac{1}{2}s[\psi_\mu^\dagger, \psi_\nu^\dagger]\partial_\mu\mathcal{K}_\nu - \frac{1}{2}s[\psi_\mu, \psi_\nu]\partial_\nu\mathcal{K}_\mu. \end{aligned} \quad (58)$$

Now suppose that we decompose the deformed $N = 1$ SUSY operator into holomorphic and antiholomorphic sectors because of $d = \partial + \bar{\partial}$. Then the G-index theorem can be associated with a high degree of symmetry on graphene molecule. Let us take a Lie group G generated by G_i which satisfies the commutation relations with Q_2 and Q_2^\dagger such that

$$[G_i, G_j] = if_{ij}^k G_k, \quad [Q_2, G_i] = 0, [Q_2^\dagger, G_i] = 0 \quad (59)$$

where f_{ij}^k mean structure constants. On graphene, there exists the Hamiltonian H such that

$$H \equiv -2\hbar^2 v_F^2 (Q_2 + Q_2^\dagger)^2, \quad [G_i, H] = 0. \quad (60)$$

On deforming Q_2 , this can be changed into a new operator

$$Q_{2s} = \psi^{\dagger\bar{z}}\partial_{\bar{z}} + s\mathcal{K}^{\bar{z}}\psi_{\bar{z}}, \quad (61)$$

where s is a real parameter. \mathcal{K} denotes a Killing vector field associated with the deformation. In the complex coordinates z and \bar{z} , the Killing vector field is given by $\mathcal{K} = -y\partial_x + x\partial_y = i(z\partial_z - \bar{z}\partial_{\bar{z}})$.

Under the deformation let us consider a graphene system corresponding to the K_+ . Then we can obtain a deformed Hamiltonian $H_{+,s}$ on the Dolbeault complex. For convenience, after replacing s by is , the deformed Hamiltonian is given by [9, 17]

$$\begin{aligned} H_{+,is} &= -2\hbar^2 v_F^2 (Q_{+,2is} + Q_{+,2is}^\dagger)^2 \\ &= -2\hbar^2 v_F^2 (-2\partial_{\bar{z}z}^2 + |s|^2|z|^2) - 2\hbar^2 v_F^2 (s[\psi^{\dagger\bar{z}}, \psi_{\bar{z}}] + s(\bar{z}\partial_{\bar{z}} - z\partial_z)). \end{aligned} \quad (62)$$

This operator gives rise to eigenvalues [9, 17]

$$E_{+,nml} = -2\hbar^2 v_F^2 \left[|s| \left(\left(n + \frac{1}{2} \right) + \left(m + \frac{1}{2} \right) + sl + s(\pm 1) \right) \right]. \quad (63)$$

Depending on the choice of $s > 0$ or $s < 0$, we can consider two cases for zero eigenvalues satisfying the topological invariance imposed by the index theorem. First if $s > 0$, we should take -1 for the $[\psi^{\dagger\bar{z}}, \psi_{\bar{z}}]$. Now we get in the bosonic sector. We can have zero eigenvalues

in the case of $l = 0, -1, -2, \dots$. Second if $s < 0$, we have to choose $+1$ for $[\psi^{\dagger\bar{z}}, \psi_{\bar{z}}]$. And then we can get zero eigenvalues for $l = 0, 1, 2, \dots$.

According to the choice of s , let us take two Hamiltonians $H_{+,is}^{\uparrow} = \widehat{Q}_{+,2is}^{\dagger} \widehat{Q}_{+,2is}$ and $H_{+,is}^{\downarrow} = \widehat{Q}_{+,2is} \widehat{Q}_{+,2is}^{\dagger}$ as two superpartners which imply the Z_2 grading over the Hilbert space. Here we have expressed $\widehat{Q}_{+,2is} = -i\sqrt{2}\hbar v_F(Q_{+,2is} + Q_{+,2is}^{\dagger})$. Then we want to calculate the eigenvalues for the up-spin and down-spin components

$$H_{+,is}^{\uparrow\downarrow} |\psi_{+,nml}^{\uparrow\downarrow}\rangle = E_{+,nml}^{\uparrow\downarrow} |\psi_{+,nml}^{\uparrow\downarrow}\rangle, \quad (64)$$

where $E_{+,n+1ml}^{\uparrow\downarrow} > E_{+,nml}^{\uparrow\downarrow} \geq E_{+,000}^{\uparrow\downarrow}$. Suppose that $E_{+,000}^{\uparrow}$ is zero. Then making use of the relations

$$\widehat{Q}_{+,i2s} H_{+,is}^{\uparrow} = \widehat{Q}_{+,2is} \widehat{Q}_{+,2is}^{\dagger} \widehat{Q}_{+,2is} = H_{+,is}^{\downarrow} \widehat{Q}_{+,2is}, \quad (65)$$

we can have

$$\begin{aligned} H_{+,is}^{\downarrow} \widehat{Q}_{+,2is} |\psi_{+,nml}^{\uparrow}\rangle &= \widehat{Q}_{+,2is} H_{+,is}^{\uparrow} |\psi_{+,nml}^{\uparrow}\rangle \\ &= E_{+,nml}^{\uparrow} \widehat{Q}_{+,2is} |\psi_{+,nml}^{\uparrow}\rangle. \end{aligned} \quad (66)$$

This means that if $E_{+,nml}^{\uparrow} \neq 0$, $\widehat{Q}_{+,2is} |\psi_{+,nml}^{\uparrow}\rangle$ is an eigenstate of $H_{+,is}^{\downarrow}$. And similarly

$$\begin{aligned} H_{+,is}^{\uparrow} \widehat{Q}_{+,2is}^{\dagger} |\psi_{+,nml}^{\downarrow}\rangle &= \widehat{Q}_{+,2is}^{\dagger} H_{+,is}^{\downarrow} |\psi_{+,nml}^{\downarrow}\rangle \\ &= E_{+,nml}^{\downarrow} \widehat{Q}_{+,2is}^{\dagger} |\psi_{+,nml}^{\downarrow}\rangle. \end{aligned} \quad (67)$$

If $E_{+,nml}^{\downarrow} \neq 0$, $\widehat{Q}_{+,2is}^{\dagger} |\psi_{+,nml}^{\downarrow}\rangle$ is an eigenstate of $H_{+,is}^{\uparrow}$. Therefore, for non-zero eigenvalues there exist the up-spin and down-spin eigenstates in pair. They form a supermultiplet connected by the supercharge $\widehat{Q}_{+,2is}$. The up-spin (down-spin) sector may be described as the bosonic (fermionic) sector at the K_+ point.

In the case of the zero eigenvalues for the down-spin sector, we should investigate both $E_{+,000}^{\downarrow} = 0$ and $E_{+,000}^{\downarrow} \neq 0$ separately. Let us assume that $E_{+,000}^{\downarrow} \neq 0$. Then the lowest eigenstate of $H_{+,is}^{\downarrow}$ is expressed as $|\psi_{+,000}^{\downarrow}\rangle \propto \widehat{Q}_{+,2is} |\psi_{+,1ml}^{\uparrow}\rangle$. Hence, there exists a supermultiplet between the states $|\psi_{+,n+1ml}^{\uparrow}\rangle$ and $|\psi_{+,nml}^{\downarrow}\rangle$, which have the same energy $E_{+,n+1ml}^{\uparrow} = E_{+,nml}^{\downarrow}$, and we obtain energy eigenstates [9]

$$\begin{aligned} |\psi_{+,nml}^{\downarrow}\rangle &= \frac{1}{\sqrt{|E_{+,n+1ml}^{\uparrow}|}} \widehat{Q}_{+,2is} |\psi_{+,n+1ml}^{\uparrow}\rangle, \\ |\psi_{+,n+1ml}^{\uparrow}\rangle &= \frac{1}{\sqrt{|E_{+,nml}^{\downarrow}|}} \widehat{Q}_{+,2is}^{\dagger} |\psi_{+,nml}^{\downarrow}\rangle \end{aligned} \quad (68)$$

for $n \geq 0$. If $E_{+,000}^\downarrow = 0$ and $\hat{Q}_{+,2is}^\dagger |\psi_{+,000}^\uparrow\rangle = 0$, the relationships are written by [9]

$$\begin{aligned} |\psi_{+,nml}^\downarrow\rangle &= \frac{1}{\sqrt{|E_{+,nml}^\uparrow|}} \hat{Q}_{+,2is} |\psi_{+,nml}^\uparrow\rangle, \\ |\psi_{+,nml}^\uparrow\rangle &= \frac{1}{\sqrt{|E_{+,nml}^\downarrow|}} \hat{Q}_{+,2is}^\dagger |\psi_{+,nml}^\downarrow\rangle \end{aligned} \quad (69)$$

for $n \geq 1$. Similarly, one can repeat eigenvalue problem for $H_{-,is}$, which corresponds to the K'_- point. As a relation between the up-spin and down-spin eigenstates, the bosonic (fermionic) sector is regarded as the down-spin (up-spin) sector at the K'_- point. And hence there exists the 4-fold degenerate energy spectrum.

VI. DEFORMED ENERGY EIGENVALUES AND UNCONVENTIONAL QUANTUM HALL EFFECT

On a sheet of graphene, let us consider the problem of magnetic field concentrated on a thin cylindrical shell of small, but finite radius $l_B = \sqrt{\frac{c\hbar}{eB}}$. The corresponding vector potential is given by $\vec{a} = (-y, x)/2l_B^2$ on the two dimensional plane of graphene. The problem in question is to compute the eigenvalues of the Dirac Hamiltonian in the field of a fractional magnetic flux on the graphene sheet [23, 24]. Now under the fractional magnetic flux, the eigenvalues for $n = 0, l = 0, m = 0$ are given by

$$\sqrt{E_{+,000}^\uparrow} = \sqrt{E_{-,000}^\downarrow} = 0, \quad (70)$$

and

$$\sqrt{E_{+,n+100}^\uparrow} = \sqrt{E_{+,n00}^\downarrow} = \sqrt{E_{-,n+100}^\downarrow} = \sqrt{E_{-,n00}^\uparrow} = \pm \hbar w_{l_B} \sqrt{n+1} \quad (71)$$

for $n \geq 0, l = 0, m = 0$. Here $w_{l_B} \equiv \frac{\sqrt{2}v_F}{l_B}$. Equation (70) tells us that there is one zero-energy state only in the case of up-spin fermions but not in the case of down-spin fermions at the K_+ point. At K'_- point we can have one zero-mode state for down-spin fermions but not for up-spin fermions. The magnetic field direction at K_+ is opposite to that at K'_- . The zero-energy state may have the four-fold degeneracy emerging from electrons and holes [8]. Since the LL of the zero-energy states becomes half-filled, no one would observe plateau at $\nu = 0$. But by index theorem, the flux quanta produce $4r$ ($r = 0, 1, 2, \dots$) zero-energy states. The $2r$ states of these are occupied. The flux quanta lift the $2r$ states to the Fermi

energy. And then they can be removed by doping. The degeneracy between electrons and holes would be removed. We could observe the Hall plateau at $\nu = 0$ because holes are occupied before electrons. And hence we can describe an experimental observation of the Hall plateau emerging at $\nu = 0$. [10]

On the basis of the index theorem, we compute the energy spectrum of the deformed Hamiltonian, $H_{+,is} = -2\hbar^2 v_F^2 (Q_{+,2is} + Q_{+,2is}^\dagger)^2$ at the K_+ point. The up-spin states of zero energy are $|0\rangle, |1\rangle, |2\rangle, \dots, |j^\uparrow - 1\rangle$. They are degenerate in $|\psi_{+,0ml}^\uparrow\rangle$. On the other hand, for down-spin states, we have to describe two cases. As the first case, assume that $j^\downarrow = 0$. Then, there do not exist any zero-energy states. So we may construct the supermultiplet given by Eq. (68). In the other case, if $j^\downarrow \neq 0$, the zero-energy states are given by $|0\rangle, |1\rangle, |2\rangle, \dots, |j^\downarrow - 1\rangle$ as degenerate states of $|\psi_{+,0ml}^\downarrow\rangle$. Therefore, these result in the $(j^\uparrow + j^\downarrow)$ -fold degeneracy in the zero-energy state for fermions at the K_+ point. This degeneracy implies the exact correspondence between j^\uparrow fermions and j^\downarrow fermions under deformation. Similarly, we can investigate the energy spectrum of the zero-energy states at the K'_- point.

In order to generate the up-spin and down-spin states of zero energy the deformed superoperators are written, in terms of the original supercharges, by

$$\widehat{Q}_{+,2is} = \widehat{Q}_{+,2is}^{\dagger j^\downarrow} \widehat{Q}_{+,2is}^{j^\uparrow}, \quad \widehat{Q}_{+,2is}^\dagger = \widehat{Q}_{+,2is}^{\dagger j^\uparrow} \widehat{Q}_{+,2is}^{j^\downarrow}, \quad (72)$$

where j^\uparrow and j^\downarrow are integers such as $j^\uparrow > j^\downarrow$. In terms of the $\widehat{Q}_{+,2is}^\dagger$ the state $|n\rangle$ is given by

$$|n\rangle = \frac{1}{\sqrt{n!}} (\widehat{Q}_{+,2is}^\dagger)^n |0\rangle. \quad (73)$$

Now, let us calculate the deformed eigenvalues by using Eq. (73) and solving the eigenvalue problems of Eq. (64) for the up-spin and down-spin components. In the bosonic sector, the deformed energy eigenvalues are expressed by

$$\sqrt{E_{+,000}^\uparrow} = \sqrt{E_{-,000}^\downarrow} = 0, \quad (74)$$

for $n = 0, l = 0, m = 0$. And we can have

$$\sqrt{E_{+,nml}^\uparrow} = \sqrt{E_{-,nml}^\downarrow} = \pm \hbar w_{l_B} \sqrt{\frac{(n + j^\uparrow - 1)!(n + j^\downarrow - 1)!}{[(n - 1)!]^2}} \quad (75)$$

for $n \geq 1, l = -(j^\uparrow - 1), m = 2(j^\uparrow - 1)$. In the case of the fermionic sector, if $j^\downarrow = 0$, the deformed eigenvalues are

$$\sqrt{E_{+,nml}^\downarrow} = \sqrt{E_{-,nml}^\uparrow} = \pm \hbar w_{l_B} \sqrt{\frac{(n+j^\downarrow)!(n+j^\uparrow)!}{[(n)!]^2}} \quad (76)$$

for $n \geq 0, l = j^\downarrow, m = 2j^\downarrow$. If $j^\downarrow \neq 0$, the eigenvalues are given by

$$\sqrt{E_{+,000}^\downarrow} = \sqrt{E_{-,000}^\uparrow} = 0, \quad (77)$$

for $n = 0, l = 0, m = 0$. And we obtain

$$\sqrt{E_{+,n+1ml}^\uparrow} = \sqrt{E_{-,n+1ml}^\downarrow} = \pm \hbar w_{l_B} \sqrt{\frac{(n+j^\downarrow-1)!(n+j^\uparrow-1)!}{[(n-1)!]^2}} \quad (78)$$

for $n \geq 1, l = j^\downarrow - 1, m = 2(j^\downarrow - 1)$. We can check up that there exists $4(j^\uparrow + j^\downarrow)$ -fold degeneracy in the zero-energy states and 4-fold one in all other states.

Among the energy spectrum given above, let us account for the special cases of $j^\uparrow = 1$, and $j^\downarrow = 0$ and $j^\uparrow = 2$, and $j^\downarrow = 0$. In the case of $j^\uparrow = 1$, and $j^\downarrow = 0$ it is not hard to check up that the energy eigenvalues are given by Eqs. (77) and (78). These results correspond to the spectrum of the monolayer graphene. For the case of $j^\uparrow = 2$, and $j^\downarrow = 0$, the energy spectra are expressed in terms of

$$\sqrt{E_{+,000}^\uparrow} = \sqrt{E_{-,000}^\downarrow} = 0, \quad (79)$$

for $n = 0, l = 0, m = 0$. And we can obtain [18]

$$\sqrt{E_{+,nml}^\uparrow} = \sqrt{E_{-,nml}^\downarrow} = \pm \hbar w_{l_B} \sqrt{n(n+1)} \quad (80)$$

for $n \geq 1, l = -1, m = 2$, while having

$$\sqrt{E_{+,nml}^\downarrow} = \sqrt{E_{-,nml}^\uparrow} = \pm \hbar w_{l_B} \sqrt{(n+1)(n+2)} \quad (81)$$

for $n \geq 0, l = 0, m = 0$. These energy spectra are eigenvalues of the bilayer graphene affected by the deformation, and are in agreement with the results in the literature [10, 12, 14]. On the basis of the index theorem we have shown that there exist the j^\uparrow -fold and j^\downarrow -degeneracy in the zero-energy state at the K_+ point and similarly at the K'_- . And hence we can obtain the QHE characterized by [9]

$$\sigma_{xy} = \nu \frac{e^2}{h}, \quad \nu = \pm 4(|n| + \frac{j^\uparrow + j^\downarrow}{2}). \quad (82)$$

VII. SUMMARY AND CONCLUSION

We presented the electronic properties of massless Dirac fermions characterized by geometry and topology on a graphene sheet in this chapter. Topological effects can be elegantly described by the Atiyah-Singer index theorem. It provides a topological invariant under deformations on the Dirac operator and plays an essential role in formulating supersymmetric quantum mechanics over twisted Dolbeault complex associated with the deformation on the topology of the lattice in a graphene system. Exploiting the G-index theorem and a high degree of symmetry, we explained deformed energy eigenvalues in graphene. The Dirac fermions result in $SU(4)$ symmetry emerging out of both the pseudospin and spin as a high degree of symmetry in the noninteracting Hamiltonian of monolayer graphene. Under the topological deformation the zero-energy states emerge naturally without the Zeeman splitting at the Fermi points in the graphene sheet. Thus we observed an emergence of a higher degree of hidden symmetry under the topological deformation in graphene while the pseudospin is a good symmetry at the K and K' points in graphene. In the particular $SU(2)$ of the pseudospin, the $SU(2)$ is the exact spin symmetry of each Landau level. In the case of nonzero energy, the up-spin and down-spin states have the exact high symmetries of spin, forming the pseudospin singlet pairing. The pseudospin can play a key role on the physics of the $n = 0$ LL in the graphene sheet. The valley pseudospin degeneracy can lift only at the zeroth LL. The 4-fold degeneracy can be removed in the zero-energy states of monolayer graphene. If the mass terms were taken into account, the four-fold degeneracy can be removed in the zero-energy state of monolayer graphene. We can exploit this to understand the emergence of a Hall plateau at $n = 0$ in the experimental observations. But the four-fold degeneracy is not removed in the higher LLs. Including the Coulomb interaction, we can lift the degeneracy. The pseudospin symmetry $SU(2)$ is broken to $U(1) \times Z_2$. Therefore the total symmetry gives rise to $SU(2)_{spin} \times (U(1) \times Z)_{pseudospin}$ while the spin symmetry $SU(2)$ remains to be exact. Hence we understood the peculiar and unconventional quantum Hall effects of the $n = 0$ Landau level in monolayer graphene on the basis of the index theorem and the high degree of symmetry under the topological deformation without the Zeeman splitting. It would be very interesting and quite possible to apply the present approach to investigation of the composite Dirac fermions and fractional quantum Hall effects in graphene.

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- [1] P. R. Wallace, Phys. Rev. **71**, 622 (1947).
 - [2] A. H. Castro Neto, et al., Rev. Mod. Phys. **81**, 109 (2009).
 - [3] K. S. Novoselov *et al.*, Science **306**, 66 (2004).
 - [4] G. W. Semenoff, Phys. Rev. Lett. **53**, 2449 (1984).
 - [5] F. D. H. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).
 - [6] K. S. Novoselov *et al.*, Nature (London) **438**, 197 (2005).
 - [7] Y. Zhang *et al.*, Nature (London)**438**, 201 (2005).
 - [8] J. K. Pachos and M. Stone, Int. J. Mod. Phys. B **21**, 5399 (2007).
 - [9] K.-S. Park *et al.*, Int. J. Mod. Phys. B,**23**, 4801 (2009); K.-S. Park *et al.*, J. Korean Phys. Soc. **50**, No 6 (2007).
 - [10] Y. Zhang *et al.*, Phys. Rev. Lett. **96**, 136806 (2006).
 - [11] K. S. Novoselov *et al.*, Nature Physics **2**, 177 (2006).
 - [12] B. E. Feldman *et al.*, Nature Phys. **5**, 889 (2009).
 - [13] Y. Zhao, Phys. Rev. Lett. **104**, 066801 (2010).
 - [14] E. McCann *et al.*, Phys. Rev. Lett. **96**, 086805 (2006).
 - [15] M. F. Atiyah and I. M. Singer, Ann. Math. **87**, 485 (1968).
 - [16] E. Witten, Nucl. Phys. B **185**, 513 (1981); Nucl. Phys. B **202**, 253 (1982); J. Differential Geometry **17**, 661 (1982).
 - [17] M. Stone, Nucl. Phys. B **314**, 557 (1989).
 - [18] M. Ezawa, Phys. Lett. B **372**, 924 (2008).
 - [19] J. González *et al.*, Nucl. Phys. B **406**, 77 (1993).
 - [20] S. Reich, C. Thomsen and P. Ordejón, Phys. Rev. B **65**, 155411 (2002).

- [21] R. Saito, M. Fujita, G. Dresselhuas, and M. S. Dresselhaus, Phys. Rev. B **46**, 1804 (1992).
- [22] T. Eguchi *et al.*, Phys. Rep. **66**, 213 (1980).
- [23] R. Jackiw and P. Rossi, Nucl. Phys. B **190**, 681 (1981).
- [24] S. Das Sarma and K. Yang, arXiv: 0906.2209v2 (2009).
- [25] S. Kim, K.-S. Park, and K. S. Yi, J. Korean Phys. Soc. **49**, S575 (2006).